SECTION I

Form Approved
O.M.B. 68-R0249

DEPARTMENT OF
HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

GRANT APPLICATION

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TYPE	PROGRAM	NUMBER
REVIEW GROUP		FORMERLY
COUNCIL *(Month, Year)*		DATE RECEIVED

TO BE COMPLETED BY PRINCIPAL INVESTIGATOR *(Items 1 through 7 and 15A)*

1. TITLE OF PROPOSAL *(Do not exceed 53 typewriter spaces)*
Resource-Related Research - Computer in Chemistry (RR-00612 renewal)

2. PRINCIPAL INVESTIGATOR

2A. NAME *(Last, First, Initial)*
Djerassi, Carl

2B. TITLE OF POSITION
Professor of Chemistry

2C. MAILING ADDRESS *(Street, City, State, Zip Code)*
Department of Chemistry
Stanford University
Stanford, CA 94305

2D. DEGREE
Ph.D.

2E. SOCIAL SECURITY NO.
[redacted]

2F. TELEPHONE DATA — Area Code: 415 — TELEPHONE NUMBER AND EXTENSION: 497-2783

2G. DEPARTMENT, SERVICE, LABORATORY OR EQUIVALENT *(See Instructions)*
Chemistry Department

2H. MAJOR SUBDIVISION *(See Instructions)*
School of Humanities and Sciences

3. DATES OF ENTIRE PROPOSED PROJECT PERIOD *(This application)*
FROM: May 1, 1980 — THROUGH: April 30, 1985

4. TOTAL DIRECT COSTS REQUESTED FOR PERIOD IN ITEM 3
$1,611,719

5. DIRECT COSTS REQUESTED FOR FIRST 12-MONTH PERIOD
$511,400

6. PERFORMANCE SITE(S) *(See Instructions)*
Stanford University
Stanford, CA 94305

7. Research Involving Human Subjects *(See Instructions)*
A. [X] NO B. [ ] YES Approved: _____ Date
C. [ ] YES – Pending Review

8. Inventions *(Renewal Applicants Only - See Instructions)*
A. [X] NO B. [ ] YES – Not previously reported
C. [ ] YES – Previously reported

TO BE COMPLETED BY RESPONSIBLE ADMINISTRATIVE AUTHORITY *(Items 8 through 13 and 15B)*

9. APPLICANT ORGANIZATION(S) *(See Instructions)*
Stanford University
Stanford, CA 94305
IRS No. 94-1156365
Congressional District 12

10. NAME, TITLE, AND TELEPHONE NUMBER OF OFFICIAL(S) SIGNING FOR APPLICANT ORGANIZATION(S)
Larry J. Lollar
Sponsored Projects Officer

Telephone Number (s) 415-497-2883

11. TYPE OF ORGANIZATION *(Check applicable item)*
[ ] FEDERAL [ ] STATE [ ] LOCAL [X] OTHER *(Specify)*
Private, non-profit university

12. NAME, TITLE, ADDRESS, AND TELEPHONE NUMBER OF OFFICIAL IN BUSINESS OFFICE WHO SHOULD ALSO BE NOTIFIED IF AN AWARD IS MADE
K. D. Creighton
Assoc. Vice President-Controller
Stanford University
Stanford, CA 94305
Telephone Number 415-497-2251

13. IDENTIFY ORGANIZATIONAL COMPONENT TO RECEIVE CREDIT FOR INSTITUTIONAL GRANT PURPOSES *(See Instructions)*

14. ENTITY NUMBER (Formerly PHS Account Number)
IRS No. 94-1156365

15. CERTIFICATION AND ACCEPTANCE. We, the undersigned, certify that the statements herein are true and complete to the best of our knowledge and accept, as to any grant awarded, the obligation to comply with Public Health Service terms and conditions in effect at the time of the award.

SIGNATURES (Signatures required on original copy only. *Use ink, "Per" signatures not acceptable)*	A. SIGNATURE OF PERSON NAMED IN ITEM 2A	DATE
	B. SIGNATURE(S) OF PERSON(S) NAMED IN ITEM 10	DATE

SECTION 1

DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

RESEARCH OBJECTIVES

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PROJECT NUMBER

NAME AND ADDRESS OF APPLICANT ORGANIZATION

Stanford University, Stanford, CA 94305

NAME, SOCIAL SECURITY NUMBER, OFFICIAL TITLE, AND DEPARTMENT OF ALL PROFESSIONAL PERSONNEL ENGAGED ON PROJECT, BEGINNING WITH PRINCIPAL INVESTIGATOR

Carl Djerassi	[redacted]	Professor of Chemistry	Department of Chemistry
Dennis H. Smith		Senior Research Associate	Department of Chemistry
Bruce G. Buchanan		Adjunct Professor	Department of Computer Science
James G. Nourse	[redacted]	Research Associate	Department of Chemistry
Neil A. B. Gray	--	Research Associate	Department of Computer Science

TITLE OF PROJECT

Resource-Related Research - Computers in Chemistry

USE THIS SPACE TO ABSTRACT YOUR PROPOSED RESEARCH. OUTLINE OBJECTIVES AND METHODS. UNDERSCORE THE KEY WORDS (NOT TO EXCEED 10) IN YOUR ABSTRACT.

Our proposed research concerns computer-assisted structure elucidation of organic compounds of biological importance. We propose to make a quantum jump in both performance of existing and new programs and their availability to a nationwide community of biomedical scientists. We will build more powerful programs (basing our efforts on the solid foundation of programs developed under earlier grant support by: a) assembling a Semi-Automated Structure Elucidation System (SASES) which will act as a computer-based "laboratory" for carrying out experiments involving computer representation and manipulation of chemical structures, including structure elucidation, spectral data interpretation and prediction and conformational analysis to establish relationships between three-dimensional structures and their biological and chemical properties (structure/property relationships); b) developing at the heart of SASES the GENOA program, a method for structure Generation with Overlapping Atoms, which will include as a component our existing CONGEN program; c) developing a method for constrained generation of molecular conformations; and d) extending our topological structure representations to include both configurational and conformational stereochemistry and infusing proper treatment of stereochemistry throughout our computer programs. We will increase the availability of our programs to the outside community through resource sharing in the following ways: a) through a dedicated computer system which will exploit the proposed relationship of our work to the SUMEX-AIM computer resource; b) by continuing to develop exportable versions of our programs; and, c) by holding intensive workshops to introduce other research groups to our techniques.

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BUDGET ESTIMATES FOR ALL YEARS OF SUPPORT REQUESTED FROM PUBLIC HEALTH SERVICE
DIRECT COSTS ONLY (Omit Cents)

DESCRIPTION		1ST PERIOD (SAME AS DETAILED BUDGET)	ADDITIONAL YEARS SUPPORT REQUESTED *(This application only)*					
			2ND YEAR	3RD YEAR	4TH YEAR	5TH YEAR	6TH YEAR	7TH YEAR
PERSONNEL COSTS		190,586	204,704	220,459	229,843	247,511		
CONSULTANT COSTS *(Include fees, travel, etc.)*								
EQUIPMENT		265,674	11,460	-	-	-		
SUPPLIES		2,600	2,782	2,977	3,185	3,408		
TRAVEL	DOMESTIC	1,500	1,500	1,500	1,500	1,500		
	FOREIGN							
PATIENT COSTS								
ALTERATIONS AND RENOVATIONS								
OTHER EXPENSES		51,040	37,836	40,483	43,320	46,351		
TOTAL DIRECT COSTS		511,400	258,282	265,419	277,848	298,770		
TOTAL FOR ENTIRE PROPOSED PROJECT PERIOD *(Enter on Page 1, Item 4)* ⟶						$ 1,611,719		

REMARKS: *Justify all costs for the first year for which the need may not be obvious. For future years, justify equipment costs, as well as any significant increases in any other category. If a recurring annual increase in personnel costs is requested, give percentage. (Use continuation page if needed.)*

Salary increases, and increases in other categories figured at 7% per year.

Staff benefits determined according to the following:

5/1/80	-	8/31/80	21.6%
9/1/80	-	8/31/81	22.4%
9/1/81	-	8/31/82	23.2%
9/1/82	-	8/31/83	24.0%
9/1/83	-	8/31/84	24.8%
9/1/84	-	4/30/85	25.6%

(see attached)

Budget Remarks

Personnel

Professor Djerassi will continue in his role as principal investigator, providing overall scientific direction to the project, Dr. Smith acting as co-investigator. Drs. Smith, Nourse, Gray and Buchanan will be responsible for the design, implementation and application of the programs which we propose to develop, including representing the scientific interface to the outside community of collaborators.

Two programmers, Mr. Terry and a person to be appointed, will provide scientific programming support for the project including the following responsibilities. Mr. Terry will have primary responsibility for maintenance and documentation of application programs, with the assistance of other members of the scientific and technical staff. He will share responsibility for design and programming of new algorithms with the scientific staff. Together with the second programmer, he will provide technical support for collaborators and be responsible for developing versions of CONGEN and newer programs for other computer systems. The second programmer, to be named, will have primary responsibility for the dedicated computer system (the DEC VAX) requested in this proposal, including interfaces to the SUMEX PDP-10 system, and all other necessary system support functions including obtaining and implementing new languages, text editors and so forth.

The pre- and postdoctoral fellows supported by the grant will be involved in applications of the programs to chemical problems in our own laboratories or in research involving development of new computer techniques in collaboration with the professional staff.

The secretarial responsibilities (105 percent of a full time person) are distributed among three persons, reflecting our best estimates of actual time spent on this grant and other grants, to myself or Prof. Feigenbaum, which support the remainder of their salaries (Ms. Learned-Driscoll is supported for the remainder of her time by the Chemistry Department).

Equipment

A Dedicated Computer System - the DEC VAX-11/780

We have requested funds in the first year of the proposal to purchase a dedicated computer system for our project. The reasons for this approach are discussed in detail in Section A.2.c, Relationship to the SUMEX-AIM Resource, and in Section C.5.a. Briefly, the implementation of this machine as an adjunct to the SUMEX resource is a research study in itself, namely, how best to provide access to computational resources in a computing environment where heavy demands are being made on both development and application of software tools for solving biomedical problems. We intend to make the dedicated system available for production use of our applications programs, assuring high quality interactive service to our collaborators. We cannot get such additional capacity for this work from SUMEX which is already overcrowded and committed to new program development rather than production use. We will exploit our close relationship with SUMEX for the development of new programs, for continued close contact with the AI community centered there, as a gateway to communication facilities allowing remote terminal

access and for sharing of peripheral equipment and operations support so far as is possible. At the end of this section we comment on our situation were the dedicated machine not approved as part of this proposal.

In considering the type of machine which could provide the needed, additional capacity, we have focussed our attention on the qualities we would require in a machine, letting these considerations guide our choice. We require high quality, interactive service to support our programs in a reasonable way. An interactive program must provide rapid response to the scientist using it. This means we need a system with a good time-sharing operating system. Our programs tend to be larger than can fit comfortably on mini-computers, and certainly the more complex programs which we propose to develop will only grow larger. This requirement suggests a system which possesses a large address space, large enough that space is not a limiting factor. The combination of time sharing and large address space suggests a virtual memory machine with demand paging. Finally, we want a machine that will maximize long-term compatibilities with the SUMEX AI community and other biochemical and chemical computing resources and laboratory systems.

We have considered several alternative computers which might meet the above qualities and would provide the needed computational power to support our community. We have rejected all 16-bit (or fewer) mini-computers on the basis of address space limitations which are too restrictive for the size of our programs. Although it is possible in principle to fit our new programs such as the exportable version of CONGEN into such a small machine using extensive overlays, the programming effort would be prohibitive.

One plausible alternative is to purchase a computer compatible with the existing DEC-10 or DEC-20 systems at SUMEX and Rutgers on which our new software such as CONGEN will run without change. There are only two reasonable alternatives here, the DEC-20 family or the Foonly F-2 (a DEC-10 compatible machine being developed by a Bay-area company). The higher end of the DEC line is prohibitively expensive (e.g., the 2040 or 2050), leaving the DEC-2020 as the only reasonable choice. These systems have the advantage of running the highly developed interactive monitors (TENEX or TOPS-20) now used at SUMEX and other AI resources. This would maximize near-term compatibility and minimize operational costs. The 2020 (and the F-2) are computationally quite slow, however, particularly for arithmetic processing since they do not have a floating point processor. We expect our new research will make significant demands in this area.

There are several other negative factors about selecting either the 2020 or the F-2. The current price-performance index of the DEC-2020 is quite poor; no price advantage per user is achieved over the much more complex (and expensive) DEC-20's. Foonly is a very small company whose future is insecure. Only a few laboratories to which we might export software and collaborate on program developments and applications operate DEC-10 or -20 compatible machines. Finally, this class of machines is rapidly becoming obsolete. DEC appears to be directing their future developments toward VAX-like machines.

In parallel with this, the ARPANET AI community has been investigating long-term alternatives for INTERLISP support given the address space limitations of the DEC-10. A number of alternatives are under consideration including a "personal" LISP machine being developed at MIT, a PRIME system being considered by BB and N (Bolt Beranek and Newman Inc.) and the DEC-VAX. It appears that a consensus is developing around VAX given its attractive architecture, good interactive operating systems (UNIX or perhaps VMS) and vendor support. The DEC-VAX also appears to be

increasingly popular in scientific laboratories, including labs of several of our workshop attendees (see Annual Report, Appendix I). As another example, the National Resource for Computation in Chemistry will soon take delivery of a VAX system, meaning that additional, chemistry related software will soon become available on the VAX. (We note that similarly configured VAX's and 2020's have similar prices; the VAX will deliver considerably more computational power, however).

In summary, purchase of a 2020 or similar machine would be an expedient, short-term option to pursue in terms of our compatibility with ourselves. We feel strongly, however, that this would be short sighted. We must look further into the future in our proposal to make the best estimate possible on the trends in computer developments followed by both manufacturers and users. We are already seeing shifts in DEC, the AI community and, most importantly, computational chemists with whom we interact, toward VAX and similar machines. It is becoming clear that VAX or its equivalent is the machine to obtain, especially as a medium for providing high quality, interactive service to our collaborators, whether by network access to Stanford or programs exported to other sites. We have, therefore, tentatively decided to purchase a VAX as the dedicated machine to support applications of our programs. The configuration of the VAX as we propose it would include:

1) Basic system, including 512 KByte memory, one RP06 disc drive, one TE16 tape drive, VMS operating system, LA120 operator console, DZ-11A for eight terminal lines ($185,000);

2) 1 MByte additional memory ($35,000);

3) Either 1 Mbyte additional memory ($35,000) or one additional RP06 disc drive ($34,000) ($35,000 figured in the total appearing on the budget)

4) FORTRAN compiler ($3,300);

5) Floating point accelerator ($9,900).

Item (2) is strongly recommended by DEC in order to support more than two or three concurrent users. The choice in item (3) remains to be made. The tradeoff here is whether or not support for a larger complement of users (8 - 12) is best handled by a separate disc system for paging, or by additional memory. Further discussions with other VAX users will be required to reach a final conclusion. The final budget figure ($254,214) was obtained by summing the above figures, taking an 11 percent educational discount and adding 6-1/2 percent California State sales tax.

We are currently evaluating the various operating systems available for the VAX, including VMS from DEC, UNIX from Bell Laboratories or the Interactive Systems Corp. UNIX version which couples both VMS and UNIX in one package. Choice of one of the non-DEC operating systems will add an additional increment to our budget. In addition, new software from DEC, such as new compilers, will represent additional costs. Given the price of the FORTRAN compiler, we can estimate other languages to cost about the same. We have requested funds in the budget to cover sortware purchases, with the greatest expense in year one.

We have also budgeted, as a one-time cost, our best estimates of the expense required to implement the SUMEX/VAX link (see Section C.5). This figure, $15,000, will cover communications interfaces, circuit boards, cabling and integrated circuits.

As a final note, the rapidly changing situation with respect to new machines and cheaper prices for existing machines may allow us to reduce these estimates in the coming months. We are making every effort to find more cost-effective ways to meet our basic goals for the dedicated computer.

We believe that a DEC maintenance contract to support the hardware is the most cost-effective way to ensure maximum computer availability for our outside collaborators. Based on the hardware cited above and DEC's standard contract prices, the cost for year one (nine-month basis, three months covered under warranty) is $13,450, including a maintenance contract on the existing GT40.

If this proposal is approved and funded without the proposed computer, we will be forced to provide access to our programs, for both development and applications, to SUMEX alone, i.e., perpetuate the current situation. Not only will an important experiment in resource access and resource sharing be lost, but our collaborators (see Section F) will become increasingly impatient at the slow response time of SUMEX. We know from past experience that if response time in a highly interactive program becomes too long, scientists will simply find more productive uses for their time and will cease to use the computer. It also must be recognized that, because SUMEX is funded separately from our grant, we must also try to ensure long-term computational support for our research. The machine configuration requested is, alone, insufficient to meet our needs in the absence of SUMEX, but would do so with augmentation (additional peripheral equipment, memory, network interface, additional terminal ports and perhaps additional personnel).

Graphics Terminals

The goals of our proposed research are heavily involved with stereochemical representations of molecular structure. The requirements for visualizing these structures plus our desires to seek improvements in the interactive capabilities of our programs (most of our collaborators have requested some form of graphic input and output) have led us to propose a low-cost alternative to expensive graphics systems (Evans and Sutherland, Vector-General) or even expensive graphics terminals like the DEC GT-40. We are currently examining alternative display systems which represent new technology and provide graphics capabilities together in some instances with capabilities for input of graphic (in our case structural) information.

We have examined several display systems so far, including those manufactured by Grinnel Systems (Santa Clara, CA), DeAnza Systems (Santa Clara, CA) and Tektronix. At this time, the Tektronix 4025 appears to have a better set of desirable features, including capacity for pseudo-rotation of structures based on sequential display of stored images, programmable functions for special graphics such as automatic construction of ring systems, and cursor control for structure input. The budget figure requested includes the basic terminal plus additional display and graphics memory (to a total of 32K and 64K bytes, respectively) to allow storage of sufficient multiple images for pseudo-rotation (to add three-dimensional characteristics to the visualized structures). We will continue to search for other low-cost graphics terminal which would meet our needs together with the needs of our collaborators.

A second terminal has been requested in the second year of the budget. By that time we should be heavily involved in representation and manipulation of three-dimensional representations of structure and would require additional graphics terminal support for program development and application.

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Carl Djerassi	Professor of Chemistry	10/29/23
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
Vienna, Austria	U. S. Citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Kenyon College	A.B.(summa cum laude)	1942	Chemistry, Biology
University of Wisconsin	Ph.D.	1945	Organic Chemistry Biochemistry (minor)

HONORS National Medal of Science ('73); Perkin Medal ('75); Am. Chem. Soc. Awards: Pure Chemistry ('58), Baekeland Medal ('59), Fritzsche Award ('60), Award for Creative Invention ('73); Freedman Foundation Patent Award ('71) and Chem. Pioneer Award ('73) of Am. Inst.Chem.; Hon. Member and Centenary Lecturer, Chem. Soc. (London); Member of National Academy of Sciences, American

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT

RESEARCH SUPPORT *(See instructions)* See page 10

HONORS (continued)

Academy of Arts and Sciences, Royal Swedish Academy of Sciences, Leopoldina, Bulgarian Academy of Sciences. Honorary D. Sc. Kenyon College, Nat. Univ. of Mexico, Federal Univ. of Rio de Janeiro, Worcester Polytechnic Inst., Wayne State, Columbia, Uppsala, Coe College, University of Geneva. Wolf Prize in Chemistry (1978), National Inventors Hall of Fame (1978).

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Academic Experience

Professor of Chemistry, Stanford University, 1959 - present
Assoc. Professor ('52-'54) and Professor ('54-'59), Wayne State University

Industrial Experience

Zoecon Corp., Palo Alto, CA, Chairman of the Board and Chief Exec. Officer, '68 - present.
Syntex Corp.: Various positions in Mexico City ('49-'52, '57-'60) and Palo Alto, CA ('60-'72) ranging from Assoc. Director of Chemical Research to President of Syntex Research.
Ciba Pharmaceutical Co., Summit, NJ, Research Chemist, '42-'43, '45-'49.

Miscellaneous

Chairman of AAAS Gordon Res. Conf. on Steroids and Nat. Prod. ('52-'54); Member Amer. Pugwash Comm. ('68-'75); Chairman, Latin American Science Board of National Academy of Sciences ('66-'68); Member ('68-'72) and Chairman ('73-'75) of Board on Science and Technology for International Development of National Academy of Sciences; Member, President's Advisory Group on Contributions of Technology to Economic Streng ('75-76); Comm. on National Medal of Science; NAS Institute of Medicine (Member of Membership Comm. ar Comm. on International Health).

Publications

Author or co-author of six books (four dealing with organic mass spectrometry(and over 930 scientific publications. The most recent publications (since January 1978) are listed here, with papers Nos. 927, 925, 924, 915, 907 and 906 being particularly relevant to this application.

☆U.S. GOVERNMENT PRINTING OFFICE: 1977—241-161:3024

RESEARCH SUPPORT: CARL DJERASSI

Since essentially all of my research is supported by the NIH, it is important for the reviewers to understand what each grant actually covers in terms of personnel, equipment, etc., and how the present renewal application of RR-00612 fits into this overall picture. Therefore, I am going into somewhat more detail than is generally required for this section.

GM-06840 (20-23): "Marine Chemistry with Special Emphasis on Steroids" 5/1/78 - 4/30/82. Current annual budget $133,042. This grant supports the bulk (equivalent to three predoctorate and five postdoctorate fellows) of my collaborators who are working on the isolation, structure elucidation, biosynthesis and possible biological function of marine steroids.

GM-20276 (05): "Magnetic Circular Dichroism of Cytochromes P-450" 7/1/78 - 6/30/79. Current budget $38,201. Aside from equipment maintenance and liquid helium, this grant supports partial salaries of two postdoctorate research associates. A renewal application, entitled "MCD of Porphyrins and Artificial Heme Proteins" has been submitted.

RR-00612 (09-10): "Resource Related Research - Computers in Chemistry" 5/1/78 - 4/30/80. Current budget $144,051 (5/1/79 - 11/30/79). The current application is for renewal of this project. The renewal represents a significant change in emphasis from the current proposal in that the SUMEX-AIM computer resource is the resource to which our research will be related in the future, rather than the mass spectrometry laboratory. For this reason, the following two (partially overlapping) applications were submitted (and are pending) for support of personnel and supplies and purchase of new equipment to maintain and upgrade the mass spectrometry laboratory. Because of this shift in emphasis, the current proposal requests no funds for support of the laboratory and does not overlap in any way with the following two proposals.

AM-04257: "Mass Spectrometry in Organic and Biochemistry" 12/1/76 - 11/30/79. Current annual budget $74,800. This grant currently supports one mass spectrometer, a senior technician to operate the instrument, one postdoctoral fellow and three predoctoral fellows, who are engaged in isolation and synthetic work related to interpretation of fragmentation patterns of known and unknown molecular structures.

A renewal application has been submitted for this grant and is currently pending. This renewal is designed to support the mass spectrometer, personnel and supplies currently supported under RR-00612. In addition funds were requested to upgrade the mass spectrometer facilities. No action has as yet been taken on this application.

Pending Application: A NIGMS Shared Instrumentation Resource proposal entitled "A Shared Mass Spectrometry Resource" has been submitted for the period 9/1/79 to 8/30/82. The first year budget is $145,046, including $130,850 of capital equipment. This proposal requests support for equipment similar to that requested in the renewal of AM-04257, with some differences reflecting the resource sharing aspects of the NIGMS program. The only personnel for whom support is requested under this proposal include 10 percent of Dr. Smith and 10 percent of a senior technicial. No action has yet been taken on this application. If AM-04257 is approved then only $18,500 is requested from NIGMS for a chemical ionization accessory.

RESEARCH SUPPORT: CARL DJERASSI (continued)

Pending Application: An application entitled "Circular Dichroism of Cyclic Ketones - Conformational Isotope Effects" with an annual budget of $55,782 for the period 4/1/79 to 3/31/81 has been submitted to the National Science Foundation. In terms of personnel, it covers the salaries of one postdoctorate and two predoctorate fellows for synthetic work on chiral ketones, whose chirality is only due to ^{13}C or deuterium. No action has as yet been taken on this application.

RECENT PUBLICATIONS

900. Magnetic Circular Dichroism Studies LII. Magnetic Circular Dichroism of Purified Forms of Rabbit Liver Cytochromes P-450 and P-420. Biochemistry 17, 33 (1978), by J. H. Dawson, J. R. Trudell, R. E. Linder, G. Barth, E. Bunnenberg and C. Djerassi.

901. Optical Rotatory Dispersion Studies CXXII. Synthesis and Circular Dichroism of (3S)-Deuteriocyclohexanone. Tetrahedron Letters, 535 (1978), by C. Djerassi, C. L. VanAntwerp and P. Sundararaman.

902. Hommes Affamés, Parasites Affamés. Prospective et Santé, No. 4, 87-91 (1978), by Carl Djerassi.

903. Marine Natural Products. Synthesis of Four Naturally Occurring 20β-H Cholanic Acid Derivatives. J. Org. Chem. 43, 1442 (1978), by D. J. Vanderah and C. Djerassi.

904. One Step Conversion of Aldehydes to Esters. Tetrahedron Letters, 1627 (1978), by P. Sundararaman, E. C. Walker and C. Djerassi.

905. Terpenoids LXXV. $\Delta^{9(12)}$-Capnellene, A New Sesquiterpene Hydrocarbon from the Soft Coral Capnella Imbricata. Tetrahedron Letters, 1671 (1978), by E. Ayanoglu, T. Gebreyesus, C. M. Beechan, C. Djerassi and M. Kaisin

906. Applications of Artificial Intelligence for Chemical Inference XXVII. Computer-Assisted Structure Manipulation. Studies in the Biosynthesis of Natural Products. Tetrahedron 34, 841 (1978), by T. H. Varkony, D. H Smith and C. Djerassi

907. Recent Advances in the Mass Spectrometry of Steroids. Pure and Appl. Chem. 50, 171 (1978), by C. Djerassi.

908. Optical Rotatory Dispersion Studies CXXIII. Experimental Evidence for Preference of Axial Deuterium over Axial Hydrogen.
J. Amer. Chem. Soc. 100, 3965 (1978)
by S.-F. Lee, G. Barth, K. Kieslich and C. Djerassi

909. Optical Rotatory Dispersion Studies CXXIV. Synthesis and Circular Dichroism of 3(S)^a- and 3(R)^e-Deuterio-4(R)-t-Butylcyclohexanone and 2(R)^a- and 2(S)^e-Deuterio-4(R)-Isopropylcyclohexanone.
Tetrahedron Letters, 2457 (1978)
by P. Sundararaman and C. Djerassi

910. Minor and Trace Sterols in Marine Invertebrates IV. Identification of Sterols with Short Side Chains in the Sponge Damiriana hawaiiana.
Helv. Chim. Acta 61, 1470 (1978)
by C. Delseth, R.M.K. Carlson, C. Djerassi, T. Erdman and P.J. Scheuer

911. "Coping with Interdependence: The Population Problem", in Proceedings of the Symposium on Energy, Food, Population and World Interdependence, Committee on Chemistry and Public Affairs, American Chemical Society, Washington, D.C., 1978, pp. 40-43; 53-55. By Carl Djerassi.

912. Minor and Trace Sterols in Marine Invertebrates V. Isolation, Structure Elucidation and Synthesis of 3β-Hydroxy-26,27-Bisnorcholest-5-en-24-one from the Sponge Psammaplysilla purpurea.
Steroids 31, 815 (1978)
by E. Ayanoglu, C. Djerassi, T. R. Erdman and P.J. Scheuer

913. Terpenoids LXXIV. The Sesquiterpenes from the Soft Coral Sinularia mayi.
Tetrahedron 34, 2503 (1978)
by C. M. Beechan, C. Djerassi and H. Eggert

914. 24-Ethyl-$\Delta^{5,24(28),28}$-cholestatrien-3β-ol - a Naturally Occurring Allenic Marine Sterol.
J. Amer.Chem. Soc. 100, 5574 (1978)
by N. Theobald, J.N. Shoolery, C. Djerassi, T.R. Erdman and P.J. Scheuer

915. Applications of Artificial Intelligence for Chemical Inference XXVIII. Computer-Assisted Simulation of Chemical Reaction Sequences. Applications to Problems of Structure Elucidation.
J. Chem. Inf. Comput. Sci. 18, 168 (1978)
by T.H. Varkony, R.E. Carhart, D.H. Smith and C. Djerassi

916. Birth Control after 1984 Revisited.
Bull. Amer. Acad. of Arts and Sciences 32, No. 1, (1978)
by C. Djerassi

917. Determination of the Absolute Configuration of Stelliferasterol and Strongylosterol - Two Marine Sterols with "Extended" Side Chains.
Tetrahedron Letters, 4369 (1978)
by N. Theobald and C. Djerassi

918. Minor and Trace Sterols in Marine Invertebrates IX. *Verongulasterol - a Marine Sterol with a Novel Side Chain Alkylation Pattern.*
Tetrahedron Letters, 4373 (1978)
by W.C.M.C. Kokke, W. H. Fenical, C. S. Pak and C. Djerassi

919. Optical Rotatory Dispersion Studies CXXVI. Synthesis and Chiroptical Properties of Cyclohexanones with Chirality Solely Due to Isotopic Substitution: $^{12}CH_3$ vs $^{13}CH_3$ and CH_3 vs CD_3
Tetrahedron Letters, 4377 (1978)
by C. S. Pak and C. Djerassi

920. Isolation and Structure of 26,27-Cycloaplysterol (Petrosterol): A Cyclopropane-Containing Marine Sterol.
Tetrahedron Letters, 4379 (1978)
by B. N. Ravi, W.C.M.C. Kokke, C. Delseth and C. Djerassi

921. Minor and Trace Sterols in Marine Invertebrates VIII. Isolation, Structure Elucidation and Partial Synthesis of Two Novel C_{30} Marine Sterols - Stelliferasterol and Isostelliferasterol.
J. Amer. Chem. Soc., 100, 7677 (1978)
by N. Theobald, R.J. Wells and C. Djerassi

922. Optical Rotatory Dispersion Studies CXXV. Independent Evidence for Preference of Axial Deuterium vs. Axial Hydrogen through Variable Temperature Circular Dichroism Spectra of (4S)-2,2-dimethyl-4-deuteriocyclohexanone and (3S)-3-deuterio-4,4-dimethylcyclohexanone.
J. Amer. Chem. Soc., 100, 8010 (1978)
by S.F. Lee, G. Barth and C. Djerassi

923. Partial Reduction of Aquomethemoglobin on a Sephadex G-25 Column as Detected by Magnetic Circular Dichroism Spectroscopy and Revised Extinction Coefficients for Aquomethemoglobin.
Analytical Biochemistry, 90, 474 (1978)
by R. E. Linder, R. Records, G. Barth, E. Bunnenberg, C. Djerassi, B. E. Hedlund, A. Rosenberg, E. S. Benson, L. Seamans and A. Moscowitz

924. Minor and Trace Sterols in Marine Invertebrates VI. Occurrence and Possible Origins of Sterols Possessing Unusually Short Hydrocarbon Side Chains
Bioorganic Chemistry, 7, 453 (1978)
by R.M.K. Carlson, S. Popov, I. Massey, C. Delseth, E. Ayanoglu, T.H. Varkony and C. Djerassi

925. A Novel Role of Computers in the Natural Products Field.
Naturwissenschaften, 66, 9 (1979)
by C. Djerassi, D. H. Smith and T. H. Varkony

926. The Synthesis of Demethylgorgosterol.
Tetrahedron Letters, 767 (1979)
by R. D. Walkup, G. D. Anderson and C. Djerassi

927. Applications of Artificial Intelligence for Chemical Inference XXIX. Exhaustive Generation of Stereoisomers for Structure Elucidation.
J. Amer. Chem. Soc., 101, 1216 (1979)
by J. G. Nourse, R. E. Carhart, D. H. Smith and C. Djerassi

928. Minor and Trace Sterols in Marine Invertebrates XI. 5α-24-Norcholestan-3β-ol and (24Z)-Stigmasta-5,7,24(28)-trien-3β-ol, Two New Marine Sterols from the Pacific Sponges Terpios Zeteki and Dysidea Herbacea.
Helv. Chim. Acta, 62, 101 (1979)
by C. Delseth, L. Tolela, P.J. Scheuer, R.J. Wells and C. Djerassi

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE (Mo., Day, Yr.)
Dennis H. Smith	Research Associate	11-12-42

PLACE OF BIRTH (City, State, Country)	PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)	SEX
New York	USA	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Massachusetts Institute of Technology Cambridge, MA	S.B.	1964	Chemistry
University of California Berkeley, CA	Ph.D.	1967	Chemistry

HONORS

Alfred P. Sloan Foundation Scholarship, NASA Predoctoral Traineeship, Phi Lambda Upsilon, Sigma Xi, Editorial Board of Journal of Chemical Information and Computer Science.

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Mass Spectrometry and Computer Applications in Chemistry	Senior Research Associate

RESEARCH SUPPORT *(See instructions)*

n/a

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1971-present	Research Associate, Stanford University, Stanford, CA
1970-1971	Visiting Scientist, University of Bristol, Bristol, England
1967-1970	Assistant Research Chemist, University of California at Berkeley, Berkeley, CA
1965-1967	NASA Pre-Doctoral Traineeship, University of California at Berkeley, Berkeley, CA

Publications: See attached list.

(32) R.E. Carhart, D.H. Smith, H. Brown, and N.S. Sridharan, "Applications of Artificial Intelligence for Chemical Inference. XVI. Computer Generation of Vertex-Graphs and Ring Systems," J. Chem. Inf. Comp. Sci., 15, 124 (1975); Erratum, Ibid., 16, 125 (1976).

(33) R.E. Carhart, S.M. Johnson, D.H. Smith, B.G. Buchanan, R.G. Dromey, and J. Lederberg, "Networking and a Collaborative Research Community: A Case Study Using the DENDRAL Programs," in Computer Networking and Chemistry, P. Lykos, Ed., American Chemical Society, Washington, D.C., 1975.

(34) R.E. Carhart, D.H. Smith, H. Brown, and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference. XVII. An Approach to Computer-Assisted Elucidation of Molecular Structure," J. Amer. Chem. Soc., 97, 5755 (1975).

(35) D.H. Smith, "The Scope of Structural Isomerism," J. Chem. Inf. Comp. Sci., 15, 203 (1975).

(36) D.H. Smith, J.P. Konopelski, and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference. XIX. Computer Generation of Ion Structures," Org. Mass Spectrom., 11, 86 (1976).

(37) B.R. Simoneit, D.H. Smith, and G. Eglinton, "Application of Real-Time Mass Spectrometric Techniques to Environmental Organic Geochemistry. I. Computerized High Resolution Mass Spectrometry and Gas Chromatography-Low Resolution Mass Spectrometry," Arch. Environ. Cont. Tox., 3, 385 (1976).

(38) R.E. Carhart and D.H. Smith, "Applications of Artificial Intelligence for Chemical Inference. XX. 'Intelligent' Use of Constraints in Computer-Assisted Structure Elucidation," Computers in Chemistry, 1, 79 (1976).

(39) C. Cheer, D.H. Smith, C. Djerassi, B. Tursch, J.C. Braekman, and D. Daloze, "Applications of Artifical Intelligence for Chemical Inference. XXI. Chemical Studies of Marine Invertebrates. XVII. The Computer-Assisted Identification of [+]-Palustrol in the Marine Organism Cespitularia sp., aff. Subvirdis," Tetrahedron, 32, 1807 (1976).

(40) B.G. Buchanan, D.H. Smith, W.C. White, R. Gritter, E.A. Feigenbaum, J. Lederberg, and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference. XXII. Automatic Rule Formation in Mass Spectrometry by Means of the Meta-DENDRAL Program," J. Amer. Chem. Soc., 98, 6168 (1976).

(41) D.H. Smith and R. E. Carhart, "Structural Isomerism of Mono- and Sesquiterpenoid Skeletons," Tetrahedron, 32, 2513 (1976).

(42) L.L. Dunham, C.A. Henrick, D.H. Smith, and C. Djerassi, "Mass Spectrometry in Structural and Stereochemical Problems. CCXLVI.

Electron Impact Induced Fragmentation of Juvenile Hormone Analogs," Org. Mass Spectrom., 11, 1120 (1976).

(43) T.H. Varkony, R.E. Carhart, and D.H. Smith, "Computer-Assisted Structure Elucidation. Modelling Chemical Reaction Sequences Used in Molecular Structure Problems," in "Computer-Assisted Organic Synthesis," W.T. Wipke and J. Howe, Eds., American Chemical Society, Washington, D.C., 1977, p. 188.

(44) "Computer-Assisted Structure Elucidation," D.H. Smith, Ed., American Chemical Society, Washington, D.C., 1977.

(45) R.E. Carhart, T.H. Varkony, and D.H. Smith, "Computer Assistance for the Structural Chemist," in "Computer-Assisted Structure Elucidation," D.H. Smith, Ed., American Chemical Society, Washington, D.C., 1977, p. 126.

(46) D.H. Smith, M. Achenbach, W.J. Yeager, P.J. Anderson, W.L. Fitch, and T.C. Rindfleisch, "Quantitative Comparison of Combined Gas Chromatographic/Mass Spectrometric Profiles of Complex Mixtures," Anal. Chem., 49, 1623 (1977).

(47) B.G. Buchanan and D.H. Smith, "Computer Assisted Chemical Reasoning," in "Computers in Chemical Education and Research," E.V. Ludena, N.H. Sabelli, and A.C. Wahl, Eds., Plenum Press, New York, N.Y., 1977, p. 401.

(48) D.H. Smith and R.E. Carhart, "Structure Elucidation Based on Computer Analysis of High and Low Resolution Mass Spectral Data," in "High Performance Mass Spectrometry: Chemical Aplications," M.L. Gross, Ed., American Chemical Society, 1978, p. 325.

(49) T.H. Varkony, D.H. Smith, and C. Djerassi, "Computer-Assisted Structure Manipulation: Studies in the Biosynthesis of Natural Products," Tetrahedron, 34, 841 (1978).

(50) D.H. Smith and P.C. Jurs, "Prediction of 13C NMR Chemical Shifts," J. Am. Chem. Soc., 100, 3316 (1978).

(51) T.H. Varkony, R.E. Carhart, D.H. Smith, and C. Djerassi, "Computer-Assisted Simulation of Chemical Reaction Sequences. Applications to Problems of Structure Elucidation," J. Chem. Inf. Comp. Sci., 18, 168 (1978).

(52) D.H. Smith, T.C. Rindfleisch, and W.J. Yeager, "Exchange of Comments: Analysis of Complex Volatile Mixtures by a Combined Gas Chromatography-Mass Spectrometry System," Anal. Chem., 50, 1585 (1978).

(53) W.L. Fitch, P.J. Anderson, and D.H. Smith, "Isolation, Identification and Quantitation of Urinary Organic Acids," J. Chrom., 162, 249 (1979).

(54) W.L. Fitch, E.T. Everhart, and D.H. Smith, "Characterization of Carbon Black Adsorbates and Artifacts Formed During Extraction," Anal. Chem., 50, 2122 (1978).

(55) W.L. Fitch and D.H. Smith, "Analysis of Adsorption Properties and Adsorbed Species on Commercial Polymeric Carbons," Environ. Sci. Tech., 13, 341 (1979).

(56) J.G. Nourse, R.E. Carhart, D.H. Smith, and C. Djerassi, "Exhaustive Generation of Stereoisomers for Structure Elucidation," J. Am. Chem. Soc., 101, 1216 (1979).

(57) C. Djerassi, D.H. Smith, and T.H. Varkony, "A Novel Role of Computers in the Natural Products Field," Naturwiss., 66, 9 (1979).

(58) N.A.B. Gray, D.H. Smith, T.H. Varkony, R.E. Carhart, and B.G. Buchanan, "Use of a Computer to Identify Unknown Compounds. The Automation of Scientific Inference," Chapter 7 in "Biomedical Applications of Mass Spectrometry," G.R. Waller, Ed., in press.

(59) T.C. Rindfleisch and D.H. Smith, in Chapter 3 of "Biomedical Applications of Mass Spectrometry," G.R. Waller, Ed., in press.

(60) T.H. Varkony, Y. Shiloach, and D.H. Smith, "Computer-Assisted Examination of Chemical Compounds for Structural Similarities," J. Chem. Inf. Comp. Sci., in press.

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE (Mo., Day, Yr.)
Buchanan, Bruce G.	Adjunct Professor of Computer Science	7/7/40
PLACE OF BIRTH (City, State, Country)	**PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)**	**SEX**
St. Louis, Missouri	U.S.	XX Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Ohio Wesleyan University, Delaware, Ohio	B.A.	1961	Mathematics
Michigan State University	M.A.	1966	Philosophy
	Ph.D.		

HONORS
Recipient of National Institutes of Health Career Development Award (1971-1976).
continued on attached sheet

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Artificial Intelligence	Principal Investigator

RESEARCH SUPPORT *(See instructions)*

NIH 5R24 RR 00612-09 Resource Related Research: Computers and Chemistry 5/1/77 to 9/30/79 Time presently committed: 20%

Dept. of Defense MDA 903-77-C-0322; Heuristic Programming 8/1/77 to 9/30/79. Time presently committed: 45%

National Science Foundation MCS 7702712 Knowledge-Based Intelligent Systems 6/1/77 to 5/30/79. Time presently committed: 10%

National Science Foundation MCS 78-02777; MOLGEN: A Computer Science Application to Molecular Genetics . Time presently committed: 25%

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1976 - present	Adjunct Professor; Computer Science Department, Stanford University, Stanford, CA 94305.
1972-1976	Research Computer Scientist, Computer Science Department, Stanford University.
1966-1971	Research Associate, Artificial Intelligence Project, Stanford University.

Selected Publications - See attached

*U.S. GOVERNMENT PRINTING OFFICE: 1977—241-161:3024

Recent Honors

Editorial Board, Artificial Intelligence: An International Journal.
Chairman of IJCAI-79 Program Committee (International Joint Conference on Artificial Intelligence, Tokyo, 1979).
Invited Speaker, Workshop on The Logic of Discovery & Diagnosis in Medicine (Pittsburgh, October 1978).
Invited Speaker, Douglass College Seminars for Faculty, (Rutgers University, 1978).

Selected Publications

Bruce G. Buchanan, G.L. Sutherland, E.A. Feigenbaum, "Toward an Understanding of Information Processes of Scientific Inference in the Context of Organic Chemistry." in B. Meltzer and D. Michie (eds.), Machine Intelligence, 5, Edinburgh: Edinburgh University Press, 1970.

J. Lederberg, G.L. Sutherland, B.G. Buchanan, E.A. Feigenbaum, A.V. Robertson, A.M. Duffield, and C. Djerassi, "Applications of Artificial Intelligence for Chemical Inference I. The Number of Possible Organic Compounds: Acyclic Structures Containing C,H,O and N," Journal of the Am. Chem. Society, 91, 2973, 1969.

C.W. Churchman and B.G. Buchanan, "On the Design of the Inductive Systems: Some Philosophical Problems," British Journal for the Philosophy of Science, 20, 311, 1969.

B.G. Buchanan, E.A. Feigenbaum, and N.S. Sridharan, "Heuristic Theory Formation: Data Interpretation and Rule Formation," in B. Meltzer and D. Michie (eds.), Machine Intelligence 7, Edinburgh: Edinburgh University Press, 1972.

D. Michie and B.G. Buchanan, "The Scientist's Apprentice," in R.A.G. Carrington (ed.), Computers for Spectroscopy, London: Adam Hilger, 1974.

E.H. Shortliffe and B.G. Buchanan, "A Model of Inexact Reasoning in Medicine," Mathematical Biosciences, 23, 351,1975.

Selected Publications (continued)

E.H. Shortliffe, R. Davis, S.C. Axline, B.G. Buchanan, C.C. Green, S.N. Cohen, "Computer-Based Consultations in Clinical Therapeutics: Explanation and Rule Acquisition Capabilities of the MYCIN System," Computers and Biomedical Research, 8, 303, 1975.

Randall Davis, Bruce Buchanan, Edward Shortliffe, "Production Rules as a Representation of a Knowledge-Based Consultation Program," Artificial Intelligence, 8,1,1977.

B.G. Buchanan, D.H. Smith, W.C. White, R.J. Gritter, E.A. Feigenbaum, J. Lederberg, and Carl Djerassi, "Application of Artificial Intelligence for Chemical Inference XXII. Automatic Rule Formation in Mass Spectrometry by Means of the Meta-DENDRAL Program," Journal of the American Chemical Society, 98, 6168, 1976.

B.G. Buchanan, R. Davis, V. Yu and S. Cohen, "Rule Based Medical Decision Making by Computer," Proceedings of MEDINFO77, Toronto, 1977.

Bruce G. Buchanan and Tom Mitchell, "Model-Directed Learning of Production Rules," in D.A. Waterman and F. Hayes-Roth (eds.), Pattern Directed Inference Systems, New York: Academic Press, 1978.

Randall Davis and Bruce G. Buchanan, "Meta-Level Knowledge: Overview and Applications," Proceedings of the Fifth IJCAI,1,920, August 1977.

Victor L. Yu, Bruce G. Buchanan, Edward H. Shortliffe, Sharon M. Wraith, Randall Davis, A. Carlisle Scott, Stanley N. Cohen, "Evaluating the Performance of a Computer-Based Consultant." Forthcoming, Computer Programs in Biomedicine, Amsterdam.

Bruce G. Buchanan, Tom M. Mitchell, Reid G. Smith and C. Richard Johnson, Dr., "Models of Learning Systems," in J. Belzer (ed.), Encyclopedia of Computer Sciences and Technology, New York: Marcel Dekker, Inc., 1978, Vol 11.

Bruce G. Buchanan and Edward A. Feigenbaum, "DENDRAL and Meta-DENDRAL: Their Applications Dimension," to appear in Artificial Intelligence, Fall 1978.

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
James G. Nourse	Research Associate	December 14, 1947

PLACE OF BIRTH *(City, State, Country)*	PRESENT NATIONALITY *(If non-U.S. citizen, indicate kind of visa and expiration date)*	SEX
Buffalo, NY	U.S. citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Columbia University, New York, NY	B.S.	1969	Chemical Engineering
California Inst. of Tech., Pasadena, CA	Ph.D.	1974	Organic Chemistry
UCLA, Los Angeles, CA	Post Doc	1973-74	Organic Chemistry
Princeton University, Princeton, NJ	Post Doc	1974-76	Organic Chemistry

HONORS

Sigma Xi, Invited Lecturer 1978 Conference on the Permutation and its Application to Chemistry and Physics, Bielefeld, Germany

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Stereochemistry, Computer Applications	Research Associate

RESEARCH SUPPORT *(See instructions)*

n/a

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Research Associate, Department of Chemistry, Stanford University, 5/79 -
Research Affiliate, Department of Computer Science, Stanford University, 8/76 to 4/79
Postdoctoral Research Associate, Department of Chemistry, Princeton University, 2/74 to 7/76
Postdoctoral Research Associate, Department of Chemistry, UCLA, 10/73 to 1/74

☆U.S. GOVERNMENT PRINTING OFFICE 1977—241-161:3024

Publications- James G. Nourse

M. G. Hutchings, J. G. Nourse, and K. Mislow, "A First Approach to the Stereochemical Analysis of Tetraarylmethanes", Tetrahedron, 30, 1525, 1974.

J. G. Nourse, "An Algebraic Description of Stereochemical Correspondence", Proceedings of the National Academy of Sciences, 72, 2285, 1975.

J. G. Nourse and K. Mislow, "Dynamic Stereochemistry of Tetraarylmethanes and Cognate Systems. The Role of the Permutation Subgroup Lattice", Journal of the American Chemical Society, 97, 4571, 1975.

J. G. Nourse and J. D. Roberts, "Nuclear Magnetic Resonance Spectroscopy. Carbon-13 Spectra of Some Macrolide Antibiotics and Derivatives. Substituent and Conformational Effects", Journal of the American Chemical Society, 97, 4584, 1975.

J. G. Nourse, "Pseudochirality", Journal of the American Chemical Society, 97, 4594, 1975.

J. G. Nourse, "Generalized Stereoisomerization Modes", Journal of the American Chemical Society, 99, 2063, 1977.

J. G. Nourse, "The Configuration Symmetry Group and its Application to Stereoisomer Generation, Specification, and Enumeration", Journal of the American Chemical Society, 101, 1210, 1979.

J. G. Nourse, P. E. Carhart, D. H. Smith, and C. Djerassi, "Exhaustive Generation of Stereoisomers for Structure Elucidation", Journal of the American Chemical Society, 101, 1216, 1979.

J. G. Nourse, "Application of the Permutation Group in Dynamic Stereochemistry" to appear in the Proceedings of the Conference on the Permutation Group and its Application to Chemistry and Physics, held at Bielefeld, Germany, 9-12 July 1978.

J. G. Nourse, "Application of the Permutation Group to Stereoisomer Generation for Computer Assisted Structure Elucidation", to appear in the Proceedings of the Conference on the Permutation Group and its Application to Chemistry and Physics, held at Bielefled, Germany, 9-12 July, 1978.

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Neil A. B. Gray	Research Associate	September 5, 1947

PLACE OF BIRTH *(City, State, Country)*	PRESENT NATIONALITY *(If non-U.S. citizen, indicate kind of visa and expiration date)*	SEX
Edinburgh, Scotland, UK	British (currently on J-1 visa, applying for H-1)	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Imperial College, London	B. S.	1968	Chemistry
University of Cambridge	M. S.	1970	Theoretical Chemistry
	M. S.	1971	Computer Science
	Ph.D.	1977	Computer Science

HONORS

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Applications of Computers to Chemistry	

RESEARCH SUPPORT *(See instructions)*

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Science Research Council/NATO research fellow. Development of programs for structure generation and analysis including new approaches to the processing of high and low resolution mass spectral data and to handling magnetic resonance data. Stanford University, 1977-1979.

Junior Research Fellowship at King's College. Work on various computer-assisted approaches to chemical structure elucidation including both rule-based and pattern-recognition methods. Part of this work being incorporated into a Ph.D. thesis for the Computer Science Department. University of Cambridge, 1973-1977.

Research Assistant in Professor Eglinton's Organic Geochemistry Unit in the School of Chemistry on an OSTI-grant (Office for Scientific and Technical Information). Design and implementation of file-search and interpretive schemes for processing low-resolution mass spectral data, work on data-communications software and creation of small, dedicated data-acquisition system on PDP-8 mini-computers. University of Bristol, 1971-1973.

M.Sc. thesis on limitations of CNDO-type semi-empirical quantum mechanical calculations. University of Cambridge, 1968-1970.

Publications:

N.A.B. Gray and A.J. Stone.
"Justifiability of the ZDO Approximation in Terms of a Power Series Expansion."
Theoret. Chim. Acta, 18, 389 (1970).

D. Field, N.A.B.Gray and P.F. Knewstubb.
"Computational Study of the Reactions between CH4 and CH4+."
J.Chem.Soc., Faraday II, 68, 852 (1972).

D.H. Smith, N.A.B. Gray, C.T. Pillinger, B.J. Kimble and G. Eglinton.
"Geochemical and environmental applications of a compound classifier based on computer analysis of low resolution mass spectra."
Advances in Organic Geochemisty 1971.
H.R.V. Gaertner and H. Wehner (Eds).
Pergammon (1972).

T.O. Gronneberg, N.A.B. Gray and G. Eglinton.
"Computer based search and retrieval system for rapid mass spectral screening of samples."
Anal. Chem., 47, 415 (1975).

N.A.B. Gray and T.O. Gronneberg.
"Programs for spectrum classification and screening of gas-chromatographic/mass-spectrometric data on a laboratory mini-computer."
Anal.Chem., 47, 419 (1975).

N.A.B. Gray.
"A program for generating empirical spectrum classification schemes."
Org. Mass Spectrom., 10, 507 (1975).

N.A.B. Gray, J.A. Zoro, T.O. Gronneberg, S.J. Gaskell, J.N. Cardoso and G. Eglinton.
"Automatic classification of mass spectra by a laboratory computer system."
Analyt. Letters, 8, 461 (1975).

N.A.B. Gray.
"Structural Interpretation of spectra."
Anal. Chem., 47, 2426 (1975).

N.A.B. Gray.
"Similarity measures for binary coded mass spectral data."
Anal. Chem., 48, 1420 (1976).

N.A.B. Gray.
"Constraints on learning machine classification methods."
Anal. Chem., 48, 2426 (1976).

N.A.B. Gray, D.H. Smith, T.H. Varkony, R.E. Carhart
and B.G. Buchanan.
"Use of a Computer to Identify Unknown Compounds:
The Automation of Scientific Inference."
Biochemical Applications of Mass Spectrometry.
G.R. Waller (Ed).
Interscience (1979 ?).